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Sommerfeld screening parameters for *K*-state of the atoms

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Abstract The acceptable range of values of the Sommerfeld screening constant σ_2, applicable for *K*-state useful in X-ray spectra, has been estimated by using the first ionisation potential of helium, the measured energies of $K\alpha$ hypersatellites and the available values of σ_2 valid for other singly ionised states of atoms. Using this range of values of σ_2 the constant σ_1 has been calculated for singly ionised *K*-state of the atoms with Z 10 to 100. The acceptability of these calculated values has been indicated by their variation with Z.

Keywords Sommerfeld screening constants, *K*-state of atoms

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Sommerfeld [1,2] had introduced two parameters σ_1 and σ_2, to incorporate the effect of orbiting electrons on the nuclear charge, as observed by any electron in the atom. Whereas σ_1 was supposed to represent the screening of nuclear charge by all the electrons other than the observer electron, σ_2 is supposed to denote the screening by the electrons lying inner to the observer electron in the atom. Notable publications reporting the values of these constants are available in literature [1–5]. In these papers, the values of σ_1 and σ_2 have been reported as applicable for observer electron lying in any subshell other than *K*-shell. In the present study, an effort has been made to estimate the values of σ_1 and σ_2 applicable for *K*-state of the atom, useful in X-ray spectra.

Calculation of σ_2.

The constant σ_2 valid for *K*-state, as mentioned above, denotes the nuclear screening by electrons inner to *K*-shell. Though there is no such electron present in the atom, yet an electron in *K*-shell reduces the binding energy of other electrons in *K*-shell, as can be observed by the first ionisation potential of He-atom. The effect so observed can be related to the total screening constant σ_1 for He-atom.

In earlier papers, it has been reported that σ_2 is a constant for a particular subshell for all the atoms of the periodic table. The value of σ_1 for helium *K*-state can be taken as a rough estimation for σ_2, valid for *K*-shell in higher atoms. This value has been calculated as follows.

According to Bohr's theory, the binding energy of an electron in n-th orbit in hydrogen atom is given by

$$E = 2mZ^2e^4/(n^2h^2) \qquad (1)$$

For He-atom, the first and second ionisation potentials are 24.6 and 54.4 eV [6] respectively.

This indicates that the *K*-state binding energy in He^+ ion can be given by the formula (1), while for He atom, it should be written as

$$E = 2m(Z-\sigma)^2e^4/(n^2h^2). \qquad (2)$$

Using the above values of ionisation potential, these expressions give a value of σ as 0.66.

Gokhale and Misra [5] have reported the values of σ_2 for L_1-state as 2.52. Nigam and Soni (7) have reported the energies of KL states of atoms. These values are very nearly given by

$$E_z(KL) = E_z(K) + E_{z+1}(L), \qquad (3)$$

where $E_z(K)$ and $E_{z+1}(L)$ are energies of *K*-state of Z-atom and of *L*-state of $Z+1$ atom respectively. Thus, the value of σ_2 as 2.52 for L_1 state can be broken up into two parts. The integral number 2 can be assigned to screening by two *K*-electrons and the additional value 0.52 can be considered

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as a contribution of other electron present in $2s$ subshell and of electrons outer to the observer electron.

Looking at the values of σ_2 for various subshells of atoms presented by Gokhale and Misra [5], it is observed that the contribution of each inner electron very slowly decreases as more and more electrons are added in the atom. It therefore, appears that the value of σ_2 for K-state in atoms with $Z > 2$ should be less than 0.66. The acceptable value of σ_2 has been calculated as described below.

Soni and Al-Abanie [8] have reported the contribution of an individual electron to nuclear screening as observed by any other electron in the same subshell of the atom. The value for $1s$ subshell does not form a part of this report, but for all other subshells, this value has been found to be nearly 0.3. In the present study, such a value for $1s$ electron has been calculated by the same method as used earlier [8]. For these calculations, the energy of the two-hole, namely K^2-state of atom have been used, which have been calculated by the combination formula

$$E(K^h_{\alpha_2}) - E(K^2) - E(KL_2{}^1P_1). \quad (4)$$

In these formulas, $E(K\alpha_2{}^h)$ denotes the energy of hypersatellite $K\alpha_2{}^h$ and $E(K^2)$ and $E(KL_2{}^1P_1)$ denote the energies of doubly ionised states of atoms mentioned in the braces. The values of $E(KL_2{}^1P_1)$ have been taken from the report by Nigam and Soni [7] and measured values of $E(K\alpha_2{}^h)$ have been taken from the latest reports published by Keski-Rahkonen and his coworkers [9–11]. In these papers, the spectra reported were measured by ionometric methods and hence are most reliable. Though the total number of elements involved in these papers [9–11] is very small (only seven), yet the value of σ_2 obtained for all these elements is very nearly same and its average has been taken as an acceptable minimum value of σ_2 for all the elements of the periodic table. The value of the contribution to σ_1 by an electron of K-shell as observed by other K-electrons, so calculated for these atoms, is found to be 0.28.

This value is in agreement with the number mentioned in the foregoing discussion, and can be taken as a first approximation of minimum value of σ_2 for K-shell, valid for all Z.

Considering the $1s$ and $2s$ subshells to be the nearest neighbours, the value 0.52 attributed to the contributions of a $2s$ electron and all outer electrons, to the screening effect for L_1 state, can be taken as upper limit for K shell also. In doing so, we have ignored the fact that while calculating σ_2 for L_1 state, there is only one electron present in $2s$ subshell, whereas there are two electrons present in this subshell when we calculate σ_2 for K-state.

Calculation of σ_1

The energy of a singly ionised state of an atom is represented by the closed formula [4–5] :

$$(\nu/R) = (Z - \sigma_1)^2/n^2 + (Z - \sigma_2)^2/n^2 + 2/\alpha^2[1 - (1 + \alpha^2(Z - \sigma_2)^2/\{n - (j + 1/2) + [j + 1/2)^2 - \alpha^2(Z - \sigma_2)^2]^{1/2}\}^2)^{-1/2}]. \quad (5)$$

In this expression, α is fine structure constant, Z is the atomic number n is principal quantum number and j is the total quantum number. Assuming σ_2 as 0.28, we have calculated σ_1 for all the atoms in K-state. The energies of K-state have been taken from the Tables of Bearden and Burr [12], and taking $\alpha = 7.297351 \times 10^{-3}$ [4,5]. The results are shown in Table 1.

To estimate the effect of any change in accepted value of σ_2 on σ_1, we have calculated σ_1 by taking σ_2 as 0.52 also. It is noted that such a vast range of σ_2 produces a very small change in the values of σ_1 as can be seen from Table 1. It therefore, can be concluded that the values of σ_1 as given in column 2 of Table 1, indicate farely well the screening effect of nuclear charge by atomic electrons other than one electron in K-shell.

Table 1. Values of σ_1 in K-shell for different values of σ_2

Z	(σ_2 = 0.28)	(σ_2 = 0.52)
10	2.02	2.02
12	2.23	2.23
14	2.40	2.40
16	2.56	2.56
18	2.71	2.71
20	2.85	2.85
22	2.99	2.99
24	3.14	3.14
26	3.29	3.29
28	3.44	3.43
30	3.58	3.58
32	3.70	3.70
34	3.82	3.81
36	3.93	3.92
38	4.04	4.03
40	4.14	4.13
42	4.25	4.24
44	4.36	4.35
46	4.47	4.46
48	4.57	4.56
50	4.67	4.65
52	4.77	4.75
54	4.85	4.83
56	4.95	4.92
58	5.04	5.02
60	5.15	5.12
62	5.26	5.22
64	5.36	5.36
66	5.47	5.43
68	5.58	5.54
70	5.69	5.65

Table 1. *(Cont'd.)*

Z	(σ_2 = 0.28)	(σ_2 = 0.52)
72	5.79	5.75
74	5.90	5.86
76	6.01	5.96
78	6.12	6.07
80	6.23	6.17
82	6.34	6.27
84	6.45	6.38
86	6.56	6.49
88	6.67	6.59
90	6.79	6.70
92	6.91	6.82
94	7.04	6.95
96	7.18	7.08
98	7.32	7.22
100	7.47	7.36

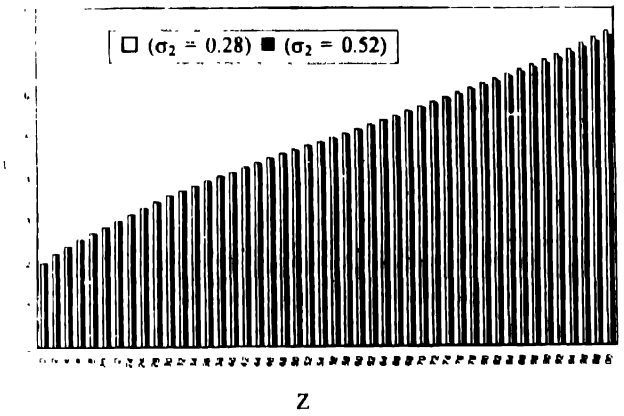

Figure 1. The variation of Sommerfeld screening parameter σ_1, for K-shell as a function of atomic number

In Figure 1, the variation in σ_1 with Z has been shown. The curve is very nearly a straight line with a positive slope equal to 0.053. Such curves for L_1, M_1 and N_1 states have been presented by Gokhale and Misra [4,5], in which the slopes are increasing as we go away from the nucleus. We observe [4,5] that the curves for L_1, M_1 are nearly straight lines with slopes equal to 0.18 and 0.35 respectively, but the curve for N_1 has still higher slope and depicts the effect of filling the d or f subshell in transition elements. As the present value of slope of σ_1 in K-shell, is lower than that for L_1 curve and also the straight line is smoother than this curve, the range of values of σ_1 presented in this study can be accepted as being the valid ones.

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